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(FILE 'HOME' ENTERED AT 11:16:37 ON 05 MAY 2008)

FILE 'REGISTRY' ENTERED AT 11:16:49 ON 05 MAY 2008

L1               STRUCTURE UPLOADED  
L2               0 S L1  
L3               52 S L1 SSS FUL  
L4               STRUCTURE UPLOADED  
L5               4 S L4 SUB=L3 FUL  
L6               27 S L3 AND CAPLUS/LC  
L7               1 S L5 AND CAPLUS/LC

FILE 'CAPLUS' ENTERED AT 11:23:41 ON 05 MAY 2008

L8               10 S L3  
L9               1 S L5  
L10              10 S L8 OR L9

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L10 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:962262 CAPLUS

DOCUMENT NUMBER: 143:248419

TITLE: Preparation of heterocyclic-fused 1,3-diazenes and analogs as metabotropic glutamate receptor antagonists

INVENTOR(S): Johansson, Martin; Wensbo, David; Minidis, Alexander; Staaf, Karin; Kers, Annika; Edwards, Louise; Isaac, Methvin; Stefanac, Tomislav; Slassi, Abdelmalik; McLeod, Donald

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; NPS Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 69 pp.

CODEN: PIXXD2

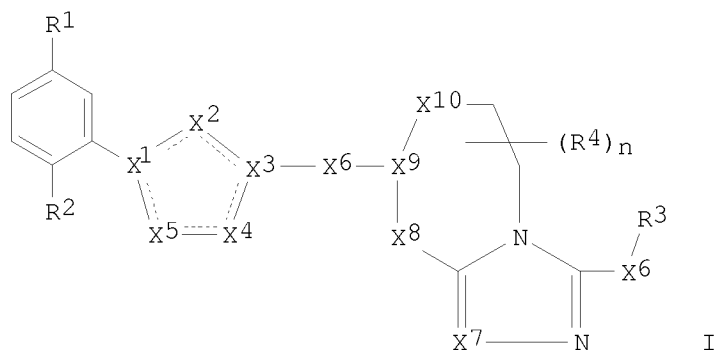
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005080397	A2	20050901	WO 2005-US5218	20050217
WO 2005080397	A3	20051222		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM			
RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2005214380	A1	20050901	AU 2005-214380	20050217
CA 2556320	A1	20050901	CA 2005-2556320	20050217
EP 1716152	A2	20061102	EP 2005-713794	20050217
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU			
CN 1934112	A	20070321	CN 2005-80008454	20050217
BR 2005007495	A	20070710	BR 2005-7495	20050217
JP 2007523183	T	20070816	JP 2006-554237	20050217
US 20060009443	A1	20060112	US 2005-60560	20050218
IN 2006DN04525	A	20070824	IN 2006-DN4525	20060804
NO 2006003562	A	20061106	NO 2006-3562	20060807
MX 2006PA09018	A	20061207	MX 2006-PA9018	20060807
US 20070185095	A1	20070809	US 2007-588699	20070309
PRIORITY APPLN. INFO.:			US 2004-545580P	P 20040219
			US 2004-545288P	P 20040218
			WO 2005-US5218	W 20050217
OTHER SOURCE(S):	MARPAT 143:248419			
GI				



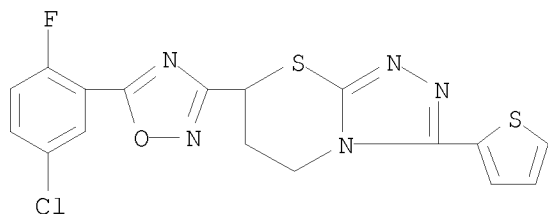
AB Title compds. I [X1-5 = C, CR5, N, O, S wherein at least one is not N; X6 = bond, divalent carbon; X7 = CR5, N; X8 = bond, divalent carbon, etc.; X9 = CR5, N; X10 = bond, divalent carbon, etc.; R1 = OH, halo, NO2, etc.; R2 = H, OH, halo, etc.; R3 = 5-6 membered ring; R4 = OH, halo, NO2, etc.; R5 = H, alkyl, cycloalkyl, aryl; n = 0-4 with some provisions] are prepared For instance, 7-[5-(5-Chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]-3-(2-thienyl)-6,7-dihydro-5H-[1,2,4]triazolo[3,4-b][1,3]thiazine is prepared by cyclization of 2-[3-[[[5-(5-chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]methyl]thio]-5-(2-thienyl)-4H-1,2,4-triazol-4-yl]ethyl methanesulfonate (DMF, NaH). Compds. of the invention have IC50 < 10  $\mu$ M for the mGluR5 receptor. I are useful for the treatment of gastrointestinal disorders.

IT 863307-58-8P, 7-[5-(5-Chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]-3-(2-thienyl)-6,7-dihydro-5H-[1,2,4]triazolo[3,4-b][1,3]thiazine  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic-fused 1,3-diazenes and analogs as metabotropic glutamate receptor antagonists)

RN 863307-58-8 CAPLUS

CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 7-[5-(5-chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]-6,7-dihydro-3-(2-thienyl)- (CA INDEX NAME)



L10 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:25972 CAPLUS

DOCUMENT NUMBER: 142:447183

TITLE: Studies on pyrazine derivatives. XL. Synthesis, reactivity, and tuberculostatic activity of 4-(hydroxyalkyl)-5-pyrazinyl-4H-[1,2,4]triazole-3-thiones

AUTHOR(S): Foks, Henryk; Janowiec, Mieczyslaw; Zwolska, Zofia; Augustynowicz-Kopec, Ewa

CORPORATE SOURCE: Department of Organic Chemistry, Medical University of Gdansk, Pol.

SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (2004), 179(12), 2519-2526  
CODEN: PSSLEC; ISSN: 1042-6507

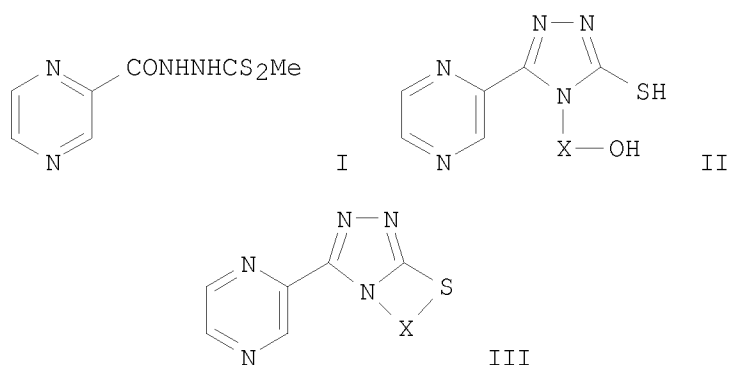
PUBLISHER: Taylor &amp; Francis, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:447183

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AB In the reactions of pyrazinoyldithiocarbazoic acid monoester (I) with amino alcs., 4-(hydroxyalkyl)-1,2,4-triazole-3-thiones [II; X = (CH<sub>2</sub>)<sub>2</sub>, (CH<sub>2</sub>)<sub>3</sub>, CH<sub>2</sub>CHMeCH<sub>2</sub>] were obtained. Their susceptibility to alkylation, as well as their heterocyclization to III (same X), were examined. Some of the compds. obtained were tested for their tuberculostatic activity.

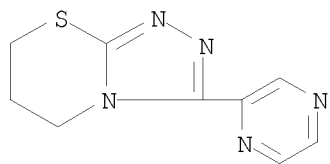
IT 717847-90-0P 851052-20-5P 851052-21-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation, alkylation, and heterocyclization of  
(hydroxyalkyl)pyrazinyltriazolethiones)

RN 717847-90-0 CAPLUS

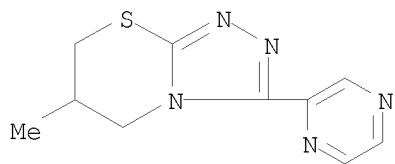
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-3-pyrazinyl- (9CI) (CA  
INDEX NAME)

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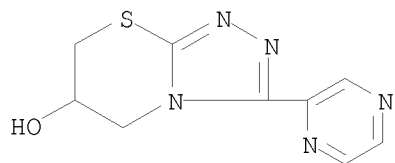
RN 851052-20-5 CAPLUS

CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-6-methyl-3-(2-pyrazinyl)- (CA INDEX NAME)



RN 851052-21-6 CAPLUS

CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-6-ol, 6,7-dihydro-3-(2-pyrazinyl)- (CA INDEX NAME)



REFERENCE COUNT:

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:356160 CAPLUS

DOCUMENT NUMBER: 138:333193

TITLE: Preparation of thien-3-yl-sulfonylamino(thio)carbonyltriazolin(thi)one derivatives as herbicides

INVENTOR(S): Gesing, Ernst-Rudolf; Drewes, Mark Wilhelm; Dahmen, Peter; Feucht, Dieter; Pontzen, Rolf

PATENT ASSIGNEE(S): Bayer CropScience AG, Germany

SOURCE: PCT Int. Appl., 104 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

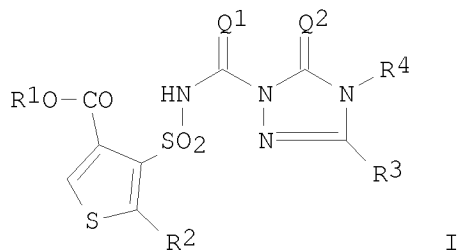
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003037086	A1	20030508	WO 2002-EP11743	20021021
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10154074	A1	20030515	DE 2001-10154074	20011102
IN 2002MU00904	A	20050121	IN 2002-MU904	20021017
CA 2465079	A1	20030508	CA 2002-2465079	20021021
AU 2002340585	A1	20030512	AU 2002-340585	20021021
EP 1443822	A1	20040811	EP 2002-774735	20021021
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002014097	A	20040928	BR 2002-14097	20021021
CN 1578625	A	20050209	CN 2002-821549	20021021
JP 2005507403	T	20050317	JP 2003-539443	20021021
RU 2316555	C2	20080210	RU 2004-116822	20021021
MX 2004PA04020	A	20040723	MX 2004-PA4020	20040428
US 20050014809	A1	20050120	US 2004-493894	20040816
PRIORITY APPLN. INFO.:			DE 2001-10154074	A 20011102
			WO 2002-EP11743	W 20021021

OTHER SOURCE(S): MARPAT 138:333193

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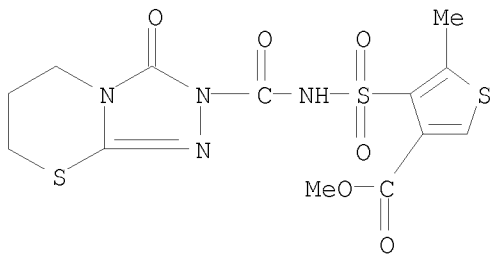
AB The thien-3-yl-sulfonylamino(thio)carbonyl-triazolin(thi)ones I [Q1, Q2 = O or S; R1 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, etc.; R2 = H, CN, NO2, halo (un)substituted alkyl, alkoxy, etc.; R3 = H, OH, SH, NH2, CN, halo, (un)substituted alkyl, alkenyl, alkynyl, etc.; R4 = H, OH, NH2, CN, alkylidenamino, (un)substituted alkyl, alkenyl, alkynyl, etc.] are prepared as herbicides. A number of known compds. are excluded.

IT 517883-79-3P 517885-09-5P 517885-48-2P

RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation as herbicide)

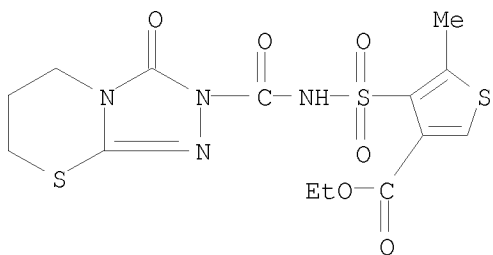
RN 517883-79-3 CAPLUS

CN 3-Thiophenecarboxylic acid, 4-[[[(6,7-dihydro-3-oxo-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-2(3H)-yl)carbonyl]amino]sulfonyl]-5-methyl-, methyl ester  
(CA INDEX NAME)



RN 517885-09-5 CAPLUS

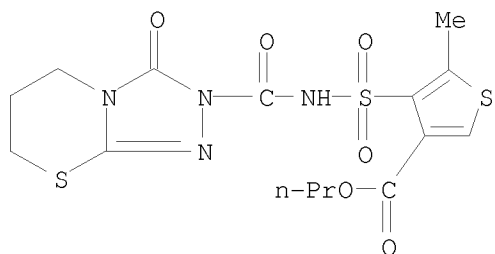
CN 3-Thiophenecarboxylic acid, 4-[[[(6,7-dihydro-3-oxo-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-2(3H)-yl)carbonyl]amino]sulfonyl]-5-methyl-, ethyl ester  
(CA INDEX NAME)



10/588,699

RN 517885-48-2 CAPLUS

CN 3-Thiophenecarboxylic acid, 4-[[[(6,7-dihydro-3-oxo-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-2(3H)-yl)carbonyl]amino]sulfonyl]-5-methyl-, propyl ester  
(CA INDEX NAME)



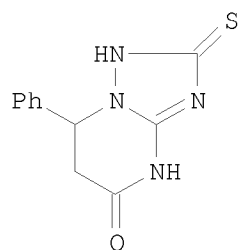
REFERENCE COUNT:

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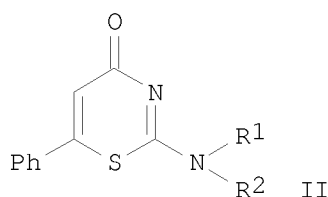
THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT



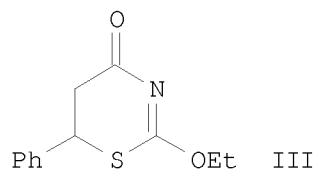
L10 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1998:598914 CAPLUS  
 DOCUMENT NUMBER: 130:81472  
 TITLE: Addition-Cyclization Reactions of Cinnamoyl  
 Isothiocyanate with Nitrogen and Oxygen Nucleophiles  
 AUTHOR(S): Ahmed, A. F. Sayed; Aouf, N.; Assy, M. G.  
 CORPORATE SOURCE: Faculty of Science, Chemistry Department, Zagazig  
 University, Zagazig, Egypt  
 SOURCE: Journal of Chemical Research, Synopses (1998), (9),  
 508-509, 2056-2061  
 CODEN: JRPSDC; ISSN: 0308-2342  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



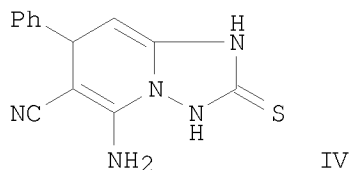
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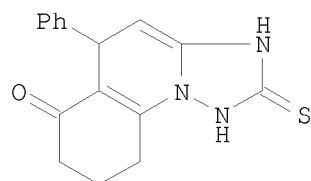
II



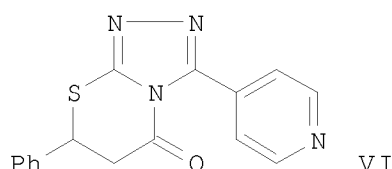
III



IV



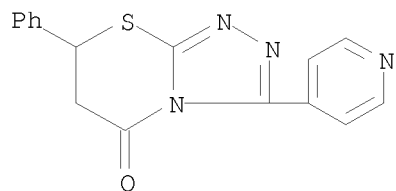
V



VI

AB Conversions of cinnamoyl isothiocyanate to heterocycles I, II (R1 = R2 = benzyl; R1 = Me, R2 = Ph), III, IV, V, and VI are described.  
 IT 218438-57-4P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (addition-cyclization reactions of cinnamoyl isothiocyanate with nitrogen and oxygen nucleophiles)  
 RN 218438-57-4 CAPLUS  
 CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 6,7-dihydro-7-phenyl-3-(4-pyridinyl)- (CA INDEX NAME)

10/588,699



REFERENCE COUNT:

9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:18718 CAPLUS

DOCUMENT NUMBER: 128:48174

TITLE: Study on the nucleophilic substitution of  
3-aryl-5-mercapto-1,2,4-triazolesAUTHOR(S): Wang, Zhong-Yi; You, Tian-Pa; Shi, Hai-Jian; Shi,  
Hao-XinCORPORATE SOURCE: Dep. Chem., Univ. Sci. Technol. China, Anhui, 230026,  
Peop. Rep. China

SOURCE: Youji Huaxue (1997), 17(6), 535-541

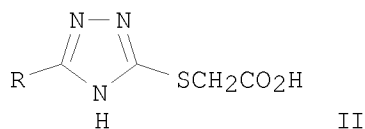
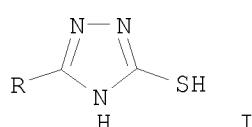
CODEN: YCHHDX; ISSN: 0253-2786

PUBLISHER: Kexue Chubanshe

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

GI



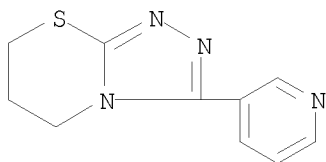
AB Reaction of title compds. I (R = Ph, 2-MeOC6H4, 2-HOC6H4, 3-O2NC6H4, 4-O2NC6H4,  $\beta$ -pyridyl) with Et bromoacetate, chloroacetic acid, 1,2-dichloroethane, and 1,3-dibromopropane were reported. E.g., reaction of I with chloroacetic acid in EtOH in the presence of NaOH gave triazoles II. II (R = Ph) showed bactericidal and anticancer activities.

IT 169517-99-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(nucleophilic substitution of 3-aryl-5-mercapto-1,2,4-triazole)

RN 169517-99-1 CAPLUS

CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-3-(3-pyridinyl)- (CA INDEX NAME)



L10 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:623169 CAPLUS

DOCUMENT NUMBER: 127:278102

TITLE: Preparation of carbapenems for use as antibacterial agents

INVENTOR(S): Miwa, Tetsuo; Soejima, Seizo

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 109 pp.

CODEN: PIXXD2

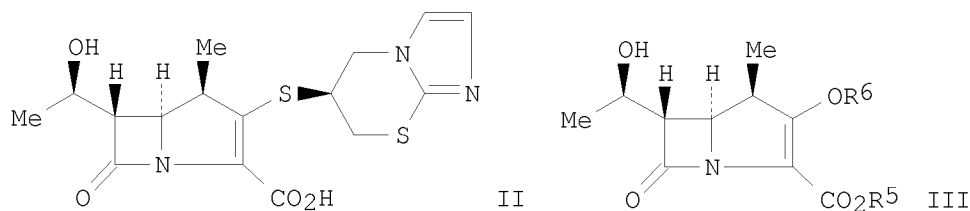
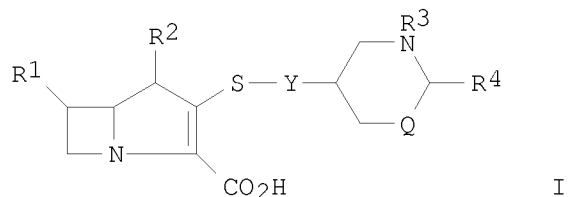
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9733888	A1	19970918	WO 1997-JP756	19970311
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GH, HU, IL, IS, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
JP 10045758	A	19980217	JP 1997-54668	19970310
AU 9722337	A	19971001	AU 1997-22337	19970311
PRIORITY APPLN. INFO.:			JP 1996-52865	A 19960311
			JP 1996-137276	A 19960530
			WO 1997-JP756	W 19970311

OTHER SOURCE(S): MARPAT 127:278102  
GI

AB Carbapenems I [R1 = substituted alkyl; R2 = H, alkyl; Y = bond, alkylene group; Q = O, S; R3R4 = nitrogen containing heterocyclic ring] were prepd and showed excellent antibacterial activities, stability, and absorbability through oral administration. Thus, the sodium salt of carbapenem II was prepared via the coupling ester III [R5 = 4-nitrobenzyl, R6 = P(O)(OPh)2] with 5-benzoylthio-6,7-dihydro-5H-imidazo[2,1-b]thiazine followed by

hydrogenation in the presence of Pd. Carbapenem II gave MIC values of 0.05 and 0.025  $\mu\text{g/mL}$  when tested against 106 CFU/mL test suspensions of *E. coli* NIHJ JC-2 and *H. influenzae* NN400 bacteria strains, resp.

IT 196602-68-3P 196602-69-4P 196602-70-7P  
196602-71-8P 196602-76-3P 196602-77-4P  
196602-78-5P 196602-79-6P

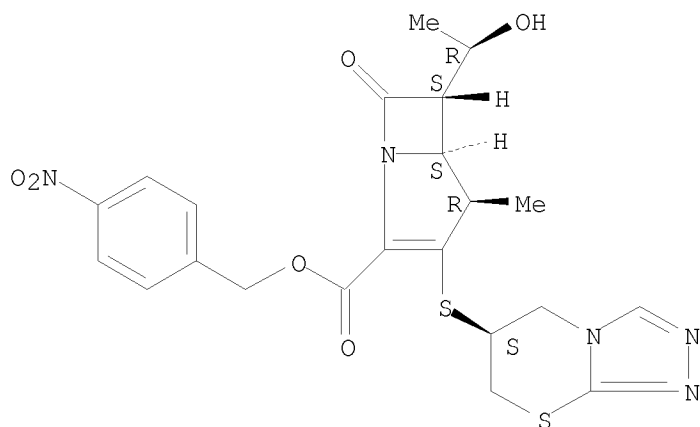
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of carbapenems for use as antibacterial agents)

RN 196602-68-3 CAPLUS

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, (4-nitrophenyl)methyl ester, [4R-[3(S\*), 4 $\alpha$ , 5 $\beta$ , 6 $\beta$ (R\*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

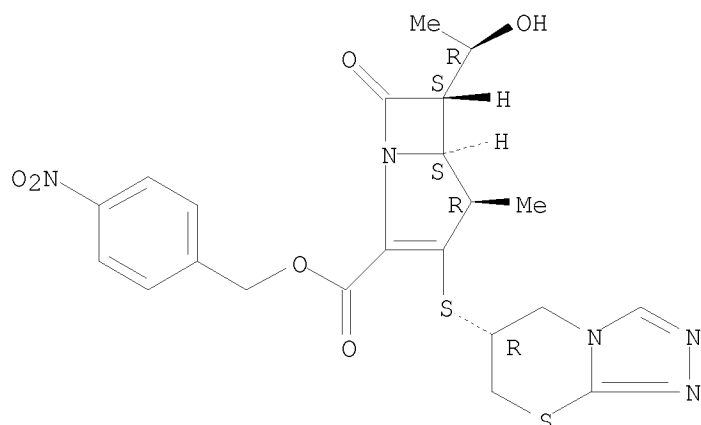


RN 196602-69-4 CAPLUS

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, (4-nitrophenyl)methyl ester, [4R-[3(R\*), 4 $\alpha$ , 5 $\beta$ , 6 $\beta$ (R\*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

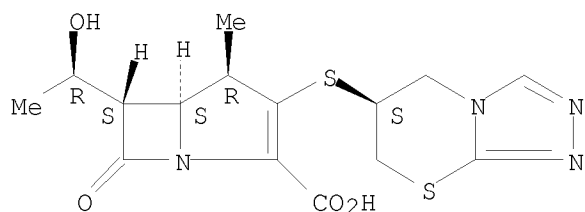
10/588,699



RN 196602-70-7 CAPLUS

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, monosodium salt, [4R-[3(S\*), 4 $\alpha$ , 5 $\beta$ , 6 $\beta$ (R\*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



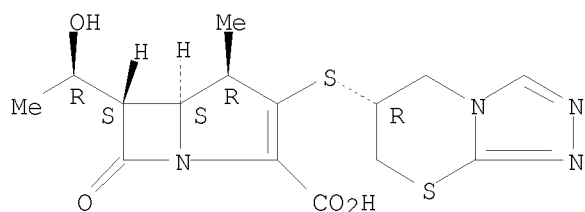
● Na

RN 196602-71-8 CAPLUS

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, monosodium salt, [4R-[3(R\*), 4 $\alpha$ , 5 $\beta$ , 6 $\beta$ (R\*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

10/588,699

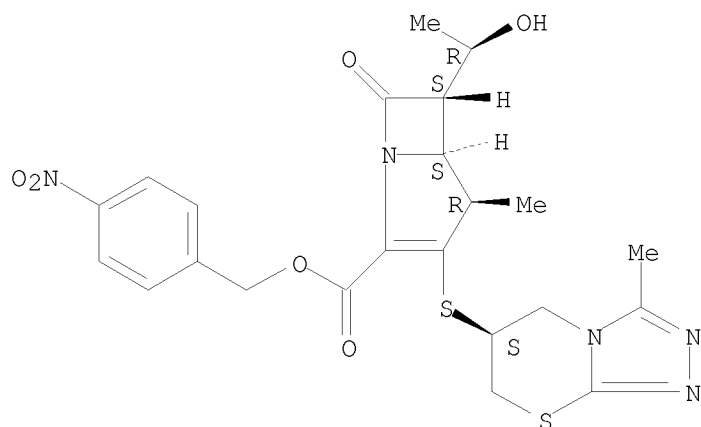


● Na

RN 196602-76-3 CAPLUS

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, (4-nitrophenyl)methyl ester, [4R-[3(S\*), 4 $\alpha$ , 5 $\beta$ , 6 $\beta$ (R\*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

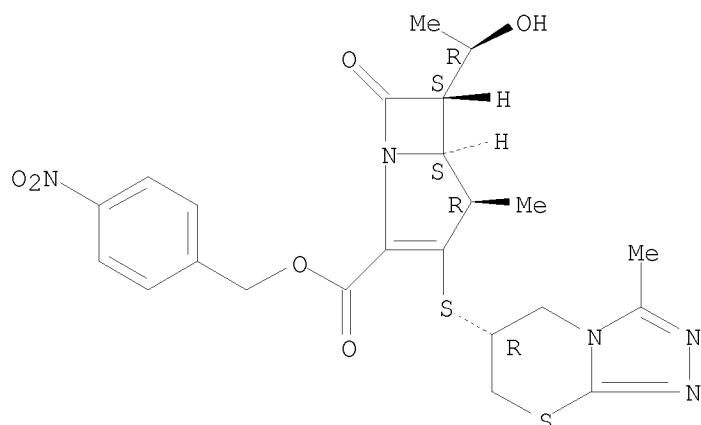


RN 196602-77-4 CAPLUS

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, (4-nitrophenyl)methyl ester, [4R-[3(R\*), 4 $\alpha$ , 5 $\beta$ , 6 $\beta$ (R\*)]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

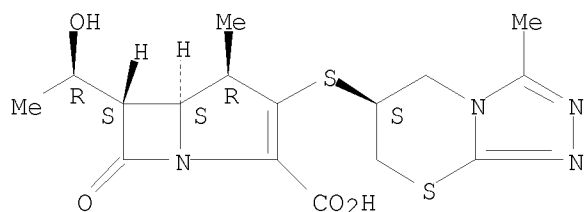
10/588,699



RN 196602-78-5 CAPLUS

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, monosodium salt, [4R-[3(S\*),4 $\alpha$ ,5 $\beta$ ,6 $\beta$ (R\*)]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



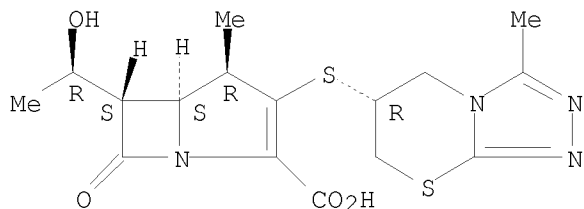
● Na

RN 196602-79-6 CAPLUS

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, monosodium salt, [4R-[3(R\*),4 $\alpha$ ,5 $\beta$ ,6 $\beta$ (R\*)]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.





● Na

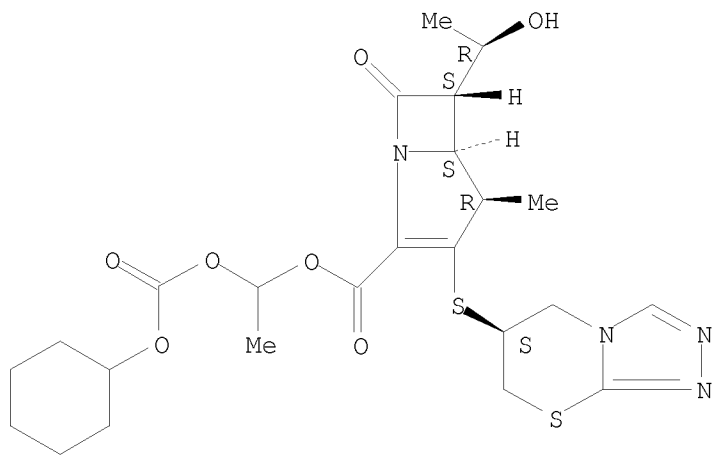
IT 196602-10-5P 196602-11-6P 196602-15-0P  
196602-16-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of carbapenems for use as antibacterial agents)

RN 196602-10-5 CAPLUS

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, 1-[[[(cyclohexyloxy)carbonyl]oxy]ethyl ester, [4R-[3(S\*), 4 $\alpha$ , 5 $\beta$ , 6 $\beta$ (R\*)]]-[partial]- (9CI) (CA INDEX NAME)

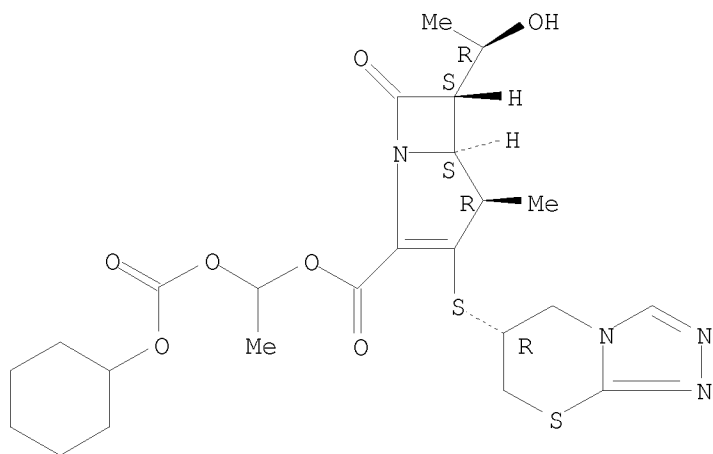
Absolute stereochemistry.



RN 196602-11-6 CAPLUS

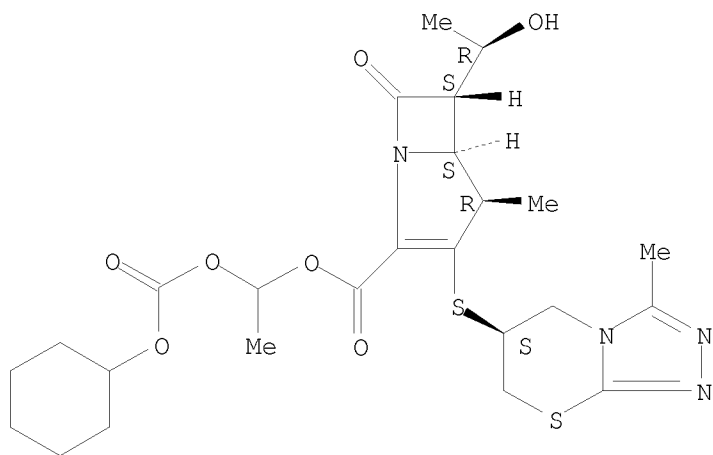
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, 1-[[[(cyclohexyloxy)carbonyl]oxy]ethyl ester, [4R-[3(R\*), 4 $\alpha$ , 5 $\beta$ , 6 $\beta$ (R\*)]]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



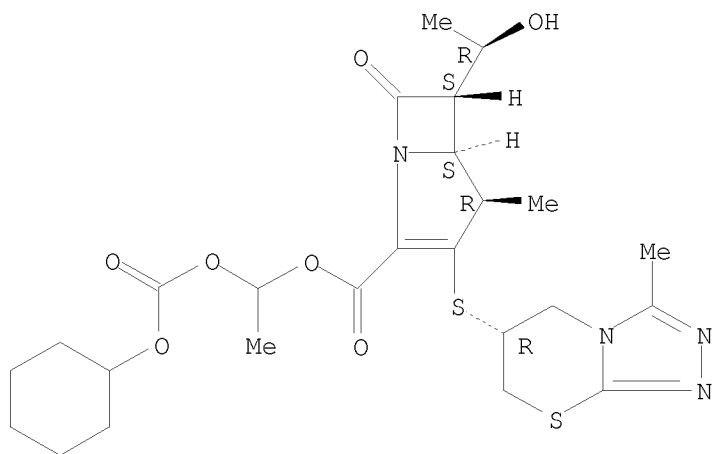
RN 196602-15-0 CAPLUS  
 CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, 1-[[[(cyclohexyloxy)carbonyl]oxy]ethyl ester, [4R-[3(S\*), 4 $\alpha$ , 5 $\beta$ , 6 $\beta$ (R\*)]]-[partial]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

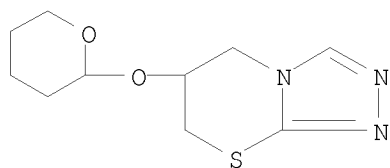


RN 196602-16-1 CAPLUS  
 CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, 1-[[[(cyclohexyloxy)carbonyl]oxy]ethyl ester, [4R-[3(R\*), 4 $\alpha$ , 5 $\beta$ , 6 $\beta$ (R\*)]]-[partial]- (9CI) (CA INDEX NAME)

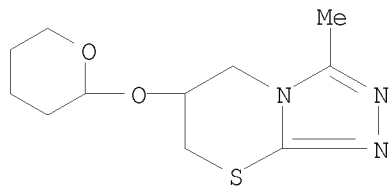
Absolute stereochemistry.



IT 196602-98-9P 196603-11-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (preparation of carbapenems for use as antibacterial agents)  
 RN 196602-98-9 CAPLUS  
 CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-6-[(tetrahydro-2H-pyran-  
 2-yl)oxy]- (CA INDEX NAME)



RN 196603-11-9 CAPLUS  
 CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-3-methyl-6-[(tetrahydro-  
 2H-pyran-2-yl)oxy]- (CA INDEX NAME)



L10 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:685539 CAPLUS

DOCUMENT NUMBER: 123:285879

TITLE: Synthesis of 2-aryl-5,6-dihydrothiazolo[2,3-c]-S-triazoles and 3-aryl-6,7-dihydro-S-triazolo[3,4-b][1,3]thiazines

AUTHOR(S): Wang, Zhongyi; Shi, Haijian; Shi, Haoxin; Zhang, Ziyi

CORPORATE SOURCE: Dep. Chem., Anhui Normal Univ., Wuhu, 241000, Peop. Rep. China

SOURCE: Huaxue Tongbao (1995), (2), 46-8

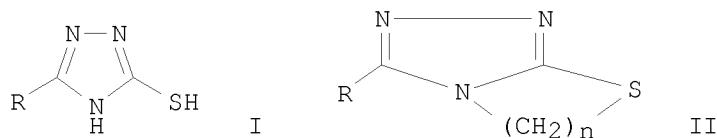
CODEN: HHTPAU; ISSN: 0441-3776

PUBLISHER: Kexue

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

GI



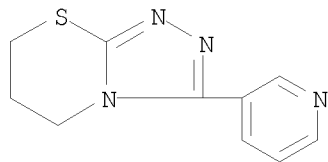
AB Reaction of triazolethiols I (R = Ph, substituted Ph, 3-pyridyl) with  $Cl(CH_2)_nCl$  ( $n = 2, 3$ ) in isopropanol in the presence of KOH- $NaHCO_3$  gave 30.9-89.2% the title compds. II.

IT 169517-99-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(synthesis of aryldihydrothiazolotriazoles and  
aryldihydrotriazolothiazines)

RN 169517-99-1 CAPLUS

CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-3-(3-pyridinyl)- (CA  
INDEX NAME)

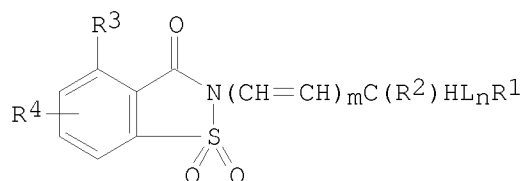


L10 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:191707 CAPLUS  
 DOCUMENT NUMBER: 120:191707  
 TITLE: 2-Substituted saccharin derivative proteolytic enzyme inhibitors  
 INVENTOR(S): Hlasta, Dennis John; Desai, Ranjit Chimanlal; Subramanyam, Chakrapani; Lodge, Eric Piatt; Dunlap, Richard Paul; Boaz, Neil Warren; Mura, Albert Joseph; Latimer, Lee Hamilton  
 PATENT ASSIGNEE(S): Sterling Winthrop Inc., USA  
 SOURCE: Eur. Pat. Appl., 77 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 7  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 542372	A1	19930519	EP 1992-203469	19921112
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
US 5236917	A	19930817	US 1991-793033	19911115
AU 9225340	A	19930520	AU 1992-25340	19920925
AU 654581	B2	19941110		
CA 2079822	A1	19930516	CA 1992-2079822	19921005
NO 9204401	A	19930518	NO 1992-4401	19921113
NO 303119	B1	19980602		
HU 66873	A2	19950130	HU 1992-3566	19921113
IL 103748	A	19970218	IL 1992-103748	19921113
RU 2101281	C1	19980110	RU 1992-4381	19921113
JP 05194444	A	19930803	JP 1992-305295	19921116
US 5371074	A	19941206	US 1993-67637	19930524
US 5650422	A	19970722	US 1994-270964	19940705
US 5596012	A	19970121	US 1995-449152	19950524
US 5874432	A	19990223	US 1997-803297	19970220
PRIORITY APPLN. INFO.:				A 19911115
				B2 19890504
				B2 19890504
				B2 19900426
				A3 19930524
				B3 19940705

OTHER SOURCE(S): MARPAT 120:191707  
 GI



AB The title compds. I [L = O, S, SO, SO<sub>2</sub>; R<sub>1</sub> = (un)substituted Ph,

(un)substituted heterocyclyl, etc.; R2 = H, lower alkoxy carbonyl, Ph, PhS; R3 = H, halogen, (un)substituted alkyl, Ph, lower alkoxy, lower alkoxy carbonyl, CN, etc.; R4 = H or 1-3 substituents selected from halogen, CN, NO2, NH2, etc.; m, n = 0, 1; when m = 0 then R1 can only be heterocyclyl and CHR2 can only be bonded to a ring N of R1; when m = 0, n = 1 and L is O, S, or SO, then R2-R4 = H; when m = 0, n = 1, L is S, R2, R4 = H and R3 = halogen; when m = 0, n = 1, and L is SO or SO2 then R2 is lower alkoxy carbonyl and R3 = R4 = H while R1  $\neq$  substituted Ph], useful for the treatment of degenerative diseases (no data), are prepared. Thus, 2-hydroxymethyl-4-chlorosaccharin was reacted with thionyl chloride, producing 2-chloromethyl-4-chlorosaccharin (II). II demonstrated inhibition constant for human leukocyte elastase (rate of reactivation of enzyme to rate of inactivation of enzyme) of 0.5 nM and 26 nM for  $\alpha$ -chymotrypsin.

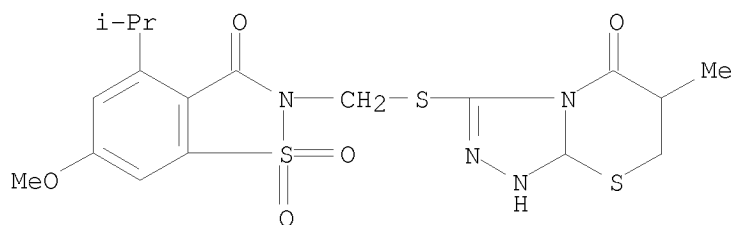
IT 152177-61-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation and proteolytic enzyme inhibitory activity of)

RN 152177-61-2 CAPLUS

CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 1,6,7,8a-tetrahydro-3-[[[6-methoxy-4-(1-methylethyl)-1,1-dioxido-3-oxo-1,2-benzisothiazol-2(3H)-yl]methyl]thio]-6-methyl- (CA INDEX NAME)



L10 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:81752 CAPLUS

DOCUMENT NUMBER: 114:81752

ORIGINAL REFERENCE NO.: 114:13957a,13960a

TITLE: Cyclization of N1-(cinnamylthiocarbamoyl)amidrazones.  
Part I

AUTHOR(S): Strzemecka, Leokadia

CORPORATE SOURCE: Inst. Bas. Chem. Sci., Sch. Med., Lublin, 20081, Pol.

SOURCE: Polish Journal of Chemistry (1990), 64(1-6), 157-66

CODEN: PJCHDQ; ISSN: 0137-5083

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:81752

AB The cyclization of R1N:CRNHNHCSNHCH2CH:CHPh (I, R = Ph, R1 = H, Ph; R = 2-pyridyl, R1 = Ph) with HCl has been studied. 1,2,4-Triazole, 1,3,4-thiadiazole, 1,2,4-triazolo[3,4-b]1,3-thiazine and 1,3,4-thiadiazolo[3,2-a]pyrimidine derivs. were obtained in good yields. With dilute HCl I (R = Ph, R1 = H) yielded both triazole and thiadiazole derivs., whereas I (R = Ph, 2-pyridyl, R1 = Ph) yielded only thiadiazoles. The cyclization reaction with concentrated HCl gave the condensed heterocycles.

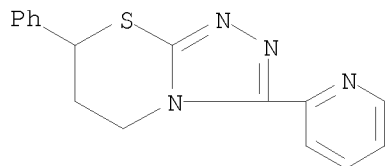
IT 132065-97-5P

RL: FORM (Formation, nonpreparative); PREP (Preparation)

(formation of, in cyclization of cinnamylthiocarbamoylamidrazone)

RN 132065-97-5 CAPLUS

CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-7-phenyl-3-(2-pyridinyl)- (CA INDEX NAME)



L10 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1980:76416 CAPLUS

DOCUMENT NUMBER: 92:76416

ORIGINAL REFERENCE NO.: 92:12587a,12590a

TITLE: A novel one-step synthesis of 3-substituted-5,6-dihydrothiazolo[2,3-c]-1,2,4-triazoles and -6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazines

AUTHOR(S): Payne, L. G.; Wu, M. T.; Patchett, A. A.

CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab. Div., Merck and Co., Inc., Rahway, NJ, 07065, USA

SOURCE: Heterocycles (1979), 12(9), 1171-4

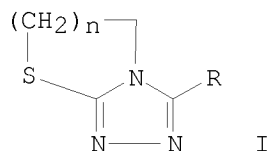
CODEN: HTCYAM; ISSN: 0385-5414

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 92:76416

GI



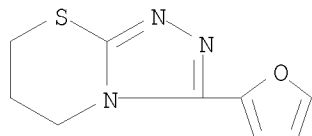
AB The title compds. I (n = 1, 2; R = 2-furyl, 4-ClC<sub>6</sub>H<sub>4</sub>, 3-pyridyl, 4-MeC<sub>6</sub>H<sub>4</sub>, Me, Pr, 3-indolylmethyl) were obtained in 35-80% yield by treating RCONHNH<sub>2</sub> with ClCH<sub>2</sub>(CH<sub>2</sub>)<sub>n</sub>NCS in the presence of NEt<sub>3</sub>.

IT 72647-26-8P 72647-34-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 72647-26-8 CAPLUS

CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 3-(2-furanyl)-6,7-dihydro- (CA INDEX NAME)

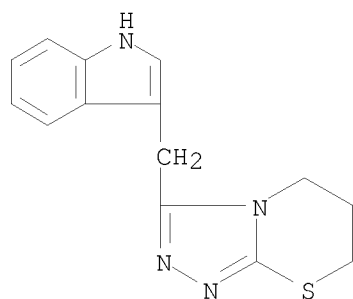


RN 72647-34-8 CAPLUS

CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 6,7-dihydro-3-(1H-indol-3-ylmethyl)- (CA INDEX NAME)



10/588,699



10/588,699

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=> s 143:248419/dn
L11      1 143:248419/DN
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=> select rn l11
ENTER ANSWER NUMBER OR RANGE (1-):1-
E1 THROUGH E60 ASSIGNED
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=> => d 115 20-25
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10/588,699

L15 ANSWER 20 OF 25 REGISTRY COPYRIGHT 2008 ACS on STN

RN 777835-35-5 REGISTRY

ED Entered STN: 10 Nov 2004

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[ (6R)-6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl]thio]-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-, (4R,5S,6S)- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, [4R-[3(R\*), 4 $\alpha$ , 5 $\beta$ , 6 $\beta$ (R\*)]]- (9CI)

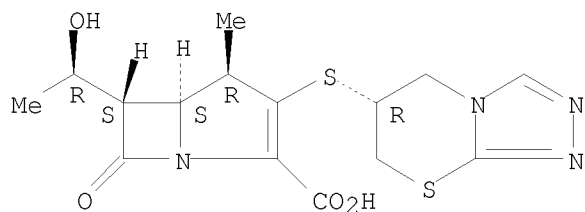
FS STEREOSEARCH

MF C15 H18 N4 O4 S2

CI COM

SR CA

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

10/588,699

L15 ANSWER 21 OF 25 REGISTRY COPYRIGHT 2008 ACS on STN

RN 774519-79-8 REGISTRY

ED Entered STN: 04 Nov 2004

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[ (6S)-6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl]thio]-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-, (4R,5S,6S)- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, [4R-[3(S\*),4 $\alpha$ ,5 $\beta$ ,6 $\beta$ (R\*)]]- (9CI)

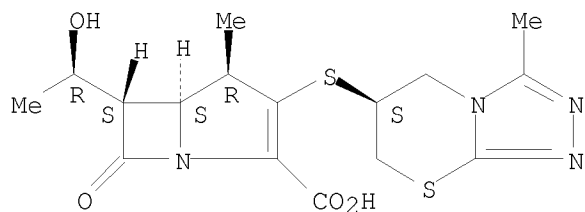
FS STEREOSEARCH

MF C16 H20 N4 O4 S2

CI COM

SR CA

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

10/588,699

L15 ANSWER 22 OF 25 REGISTRY COPYRIGHT 2008 ACS on STN

RN 764629-48-3 REGISTRY

ED Entered STN: 17 Oct 2004

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[ (6R)-6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl]thio]-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-, (4R,5S,6S)- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[(6,7-dihydro-3-methyl-5H-1,2,4-triazolo[3,4-b][1,3]thiazin-6-yl)thio]-6-(1-hydroxyethyl)-4-methyl-7-oxo-, [4R-[3(R\*),4 $\alpha$ ,5 $\beta$ ,6 $\beta$ (R\*)]]- (9CI)

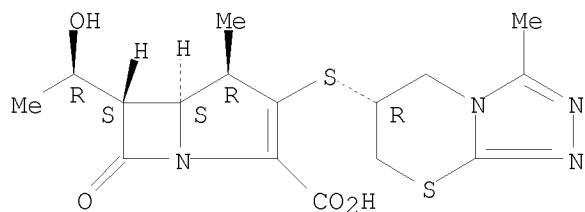
FS STEREOSEARCH

MF C16 H20 N4 O4 S2

CI COM

SR CA

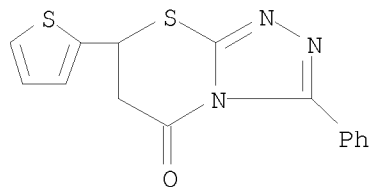
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

10/588,699

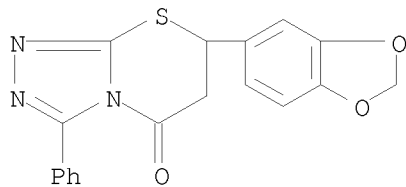
L15 ANSWER 23 OF 25 REGISTRY COPYRIGHT 2008 ACS on STN  
RN 327094-22-4 REGISTRY  
ED Entered STN: 14 Mar 2001  
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 6,7-dihydro-3-phenyl-7-(2-thienyl)- (CA INDEX NAME)  
MF C15 H11 N3 O S2  
SR Chemical Library  
Supplier: Oak Samples Ltd.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

10/588,699

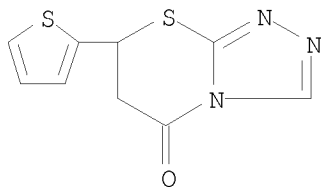
L15 ANSWER 24 OF 25 REGISTRY COPYRIGHT 2008 ACS on STN  
RN 327094-16-6 REGISTRY  
ED Entered STN: 14 Mar 2001  
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 7-(1,3-benzodioxol-5-yl)-6,7-  
dihydro-3-phenyl- (CA INDEX NAME)  
MF C18 H13 N3 O3 S  
SR Chemical Library  
Supplier: Oak Samples Ltd.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

10/588,699

L15 ANSWER 25 OF 25 REGISTRY COPYRIGHT 2008 ACS on STN  
RN 325693-79-6 REGISTRY  
ED Entered STN: 05 Mar 2001  
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 6,7-dihydro-7-(2-thienyl)-  
(CA INDEX NAME)  
MF C9 H7 N3 O S2  
SR Chemical Library  
Supplier: Oak Samples Ltd.  
LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

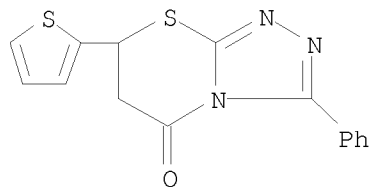


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10/588,699

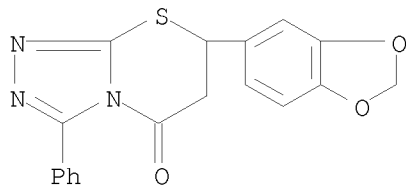
L16 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN  
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ED Entered STN: 14 Mar 2001  
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 6,7-dihydro-3-phenyl-7-(2-thienyl)- (CA INDEX NAME)  
MF C15 H11 N3 O S2  
SR Chemical Library  
Supplier: Oak Samples Ltd.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

10/588,699

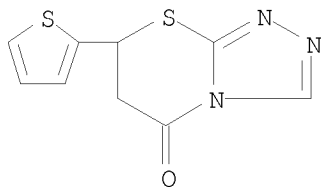
L16 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN  
RN 327094-16-6 REGISTRY  
ED Entered STN: 14 Mar 2001  
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 7-(1,3-benzodioxol-5-yl)-6,7-  
dihydro-3-phenyl- (CA INDEX NAME)  
MF C18 H13 N3 O3 S  
SR Chemical Library  
Supplier: Oak Samples Ltd.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

10/588,699

L16 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2008 ACS on STN  
RN 325693-79-6 REGISTRY  
ED Entered STN: 05 Mar 2001  
CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazin-5-one, 6,7-dihydro-7-(2-thienyl)-  
(CA INDEX NAME)  
MF C9 H7 N3 O S2  
SR Chemical Library  
Supplier: Oak Samples Ltd.  
LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

10/588,699

=> => d his

(FILE 'HOME' ENTERED AT 11:16:37 ON 05 MAY 2008)

FILE 'REGISTRY' ENTERED AT 11:16:49 ON 05 MAY 2008

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L2               0 S L1  
L3               52 S L1 SSS FUL  
L4               STRUCTURE UPLOADED  
L5               4 S L4 SUB=L3 FUL  
L6               27 S L3 AND CAPLUS/LC  
L7               1 S L5 AND CAPLUS/LC

FILE 'CAPLUS' ENTERED AT 11:23:41 ON 05 MAY 2008

L8               10 S L3  
L9               1 S L5  
L10               10 S L8 OR L9  
L11               1 S 143:248419/DN  
                  SELECT RN L11 1-

FILE 'REGISTRY' ENTERED AT 11:24:57 ON 05 MAY 2008

L12               60 S E1-60  
L13               19 S L12 AND (5-5/SZ OR 5-6/SZ OR 5-7/SZ)  
L14               41 S L12 NOT L13  
L15               25 S L3 NOT L6  
L16               3 S L5 NOT L7

FILE 'CAPLUS' ENTERED AT 11:27:30 ON 05 MAY 2008

=> s 113

L17               6 L13

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L17 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:962262 CAPLUS

DOCUMENT NUMBER: 143:248419

TITLE: Preparation of heterocyclic-fused 1,3-diazenes and analogs as metabotropic glutamate receptor antagonists

INVENTOR(S): Johansson, Martin; Wensbo, David; Minidis, Alexander; Staaf, Karin; Kers, Annika; Edwards, Louise; Isaac, Methvin; Stefanac, Tomislav; Slassi, Abdelmalik; McLeod, Donald

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; NPS Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 69 pp.

CODEN: PIXXD2

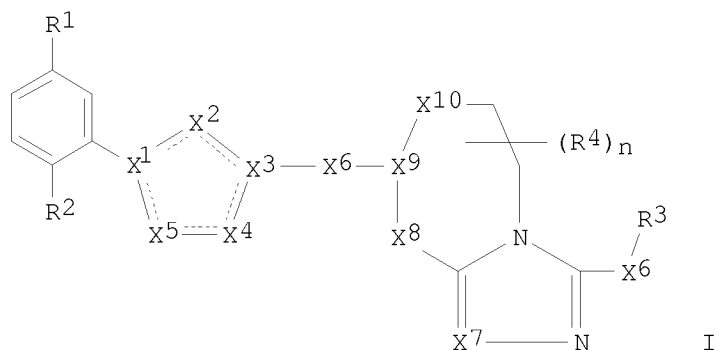
DOCUMENT TYPE: Patent

LANGUAGE: English

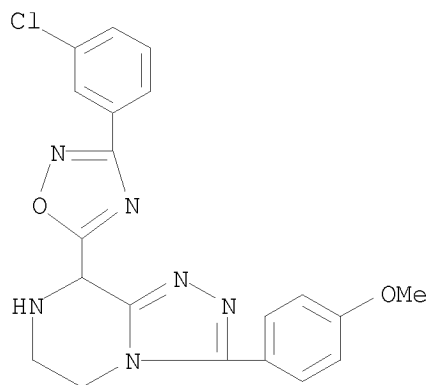
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005080397	A2	20050901	WO 2005-US5218	20050217
WO 2005080397	A3	20051222		
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RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
AU 2005214380	A1	20050901	AU 2005-214380	20050217
CA 2556320	A1	20050901	CA 2005-2556320	20050217
EP 1716152	A2	20061102	EP 2005-713794	20050217
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU			
CN 1934112	A	20070321	CN 2005-80008454	20050217
BR 2005007495	A	20070710	BR 2005-7495	20050217
JP 2007523183	T	20070816	JP 2006-554237	20050217
US 20060009443	A1	20060112	US 2005-60560	20050218
IN 2006DN04525	A	20070824	IN 2006-DN4525	20060804
NO 2006003562	A	20061106	NO 2006-3562	20060807
MX 2006PA09018	A	20061207	MX 2006-PA9018	20060807
US 20070185095	A1	20070809	US 2007-588699	20070309
PRIORITY APPLN. INFO.:			US 2004-545580P	P 20040219
			US 2004-545288P	P 20040218
			WO 2005-US5218	W 20050217
OTHER SOURCE(S):	MARPAT 143:248419			
GI				



- AB Title compds. I [X1-5 = C, CR5, N, O, S wherein at least one is not N; X6 = bond, divalent carbon; X7 = CR5, N; X8 = bond, divalent carbon, etc.; X9 = CR5, N; X10 = bond, divalent carbon, etc.; R1 = OH, halo, NO<sub>2</sub>, etc.; R2 = H, OH, halo, etc.; R3 = 5-6 membered ring; R4 = OH, halo, NO<sub>2</sub>, etc.; R5 = H, alkyl, cycloalkyl, aryl; n = 0-4 with some provisions] are prepared For instance, 7-[5-(5-Chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]-3-(2-thienyl)-6,7-dihydro-5H-[1,2,4]triazolo[3,4-b][1,3]thiazine is prepared by cyclization of 2-[3-[[[5-(5-chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]methyl]thio]-5-(2-thienyl)-4H-1,2,4-triazol-4-yl]ethyl methanesulfonate (DMF, NaH). Compds. of the invention have IC<sub>50</sub> < 10 μM for the mGluR5 receptor. I are useful for the treatment of gastrointestinal disorders.
- IT 863307-72-6P, 8-[3-(3-Chlorophenyl)-[1,2,4]oxadiazol-5-yl]-3-(4-methoxyphenyl)-5,6,7,8-tetrahydro-[1,2,4]triazolo[4,3-a]pyrazine  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of heterocyclic-fused 1,3-diazenes and analogs as metabotropic glutamate receptor antagonists)
- RN 863307-72-6 CAPLUS
- CN 1,2,4-Triazolo[4,3-a]pyrazine, 8-[3-(3-chlorophenyl)-1,2,4-oxadiazol-5-yl]-5,6,7,8-tetrahydro-3-(4-methoxyphenyl)- (CA INDEX NAME)



- IT 863307-58-8P, 7-[5-(5-Chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]-3-(2-thienyl)-6,7-dihydro-5H-[1,2,4]triazolo[3,4-b][1,3]thiazine

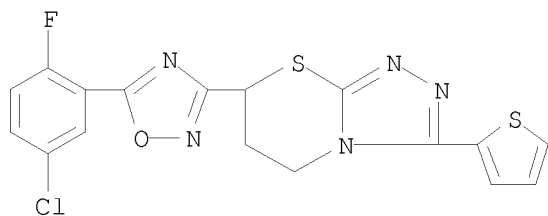
863307-59-9P, 9-[[5-(3-Chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(pyridin-4-yl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-60-2P, 9-[[5-(3-Chlorophenyl)isoxazol-3-yl]methyl]-3-(3,5-difluorophenyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-61-3P, 9-[[5-(3-Chlorophenyl)isoxazol-3-yl]methyl]-3-(4-methoxyphenyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-63-5P, 9-[[5-(3-Chlorophenyl)isoxazol-3-yl]methyl]-3-(pyridin-4-yl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-65-7P, 9-[[5-(5-Chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(pyridin-4-yl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-66-8P, 9-[[5-(3-Chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(3,5-difluorophenyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-68-0P, 9-[[5-(3-Chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(4-methoxyphenyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-69-1P, 9-[1-[5-(3-Chlorophenyl)-1,2,4-oxadiazol-3-yl]ethyl]-3-(pyridin-4-yl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-70-4P, 7-[[5-(3-Chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(pyridin-4-yl)-6,7-dihydro-5H-pyrrolo[2,1-c][1,2,4]triazole 863307-71-5P, 9-[[5-(3-Chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(trifluoromethyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-73-7P, 8-[3-(3-Chlorophenyl)-[1,2,4]oxadiazol-5-yl]-3-(4-methoxyphenyl)-7-methyl-5,6,7,8-tetrahydro-[1,2,4]triazolo[4,3-a]pyrazine

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic-fused 1,3-diazenes and analogs as metabotropic glutamate receptor antagonists)

RN 863307-58-8 CAPLUS

CN 5H-1,2,4-Triazolo[3,4-b][1,3]thiazine, 7-[5-(5-chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]-6,7-dihydro-3-(2-thienyl)- (CA INDEX NAME)

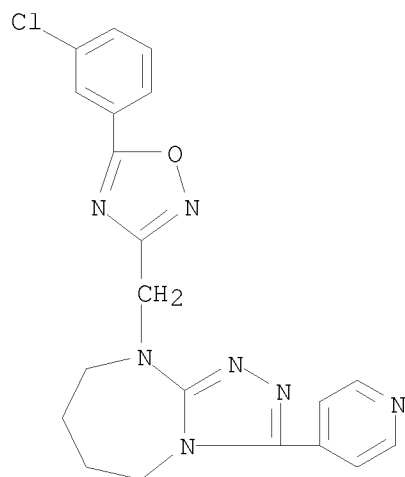


RN 863307-59-9 CAPLUS

CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(3-chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-6,7,8,9-tetrahydro-3-(4-pyridinyl)- (CA INDEX NAME)

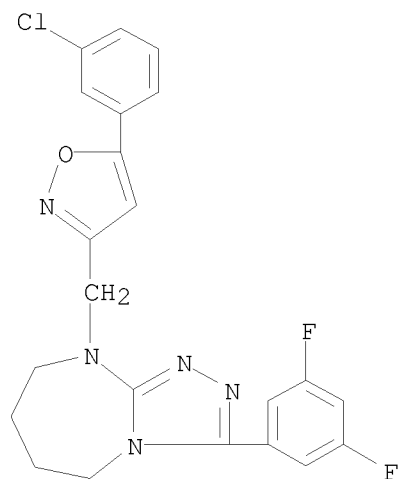


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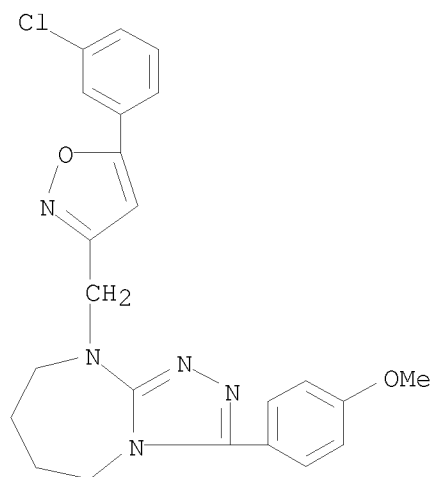
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(3-chlorophenyl)-3-isoxazolyl]methyl]-3-(3,5-difluorophenyl)-6,7,8,9-tetrahydro- (CA INDEX NAME)



RN 863307-61-3 CAPLUS

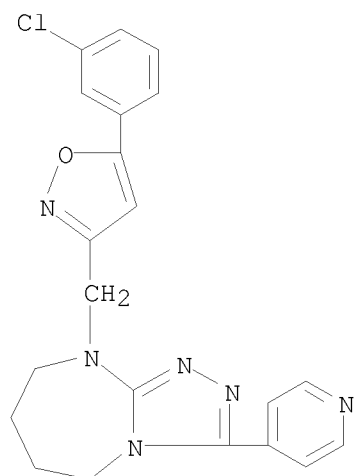
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(3-chlorophenyl)-3-isoxazolyl]methyl]-6,7,8,9-tetrahydro-3-(4-methoxyphenyl)- (CA INDEX NAME)

10/588,699



RN 863307-63-5 CAPLUS

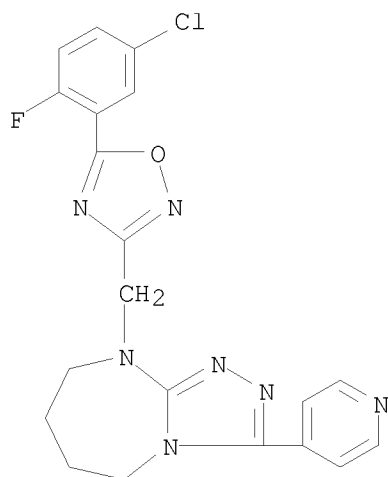
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(3-chlorophenyl)-3-isoxazolyl]methyl]-6,7,8,9-tetrahydro-3-(4-pyridinyl)- (CA INDEX NAME)



RN 863307-65-7 CAPLUS

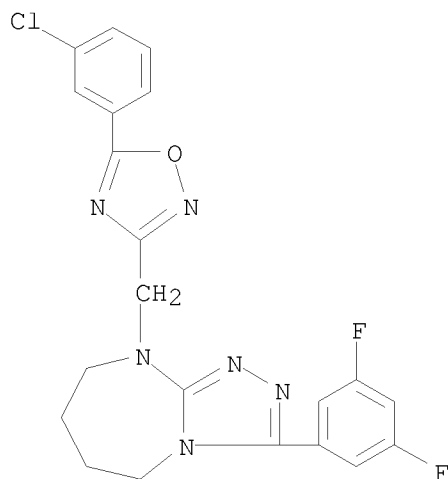
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(5-chloro-2-fluorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-6,7,8,9-tetrahydro-3-(4-pyridinyl)- (CA INDEX NAME)

10/588,699



RN 863307-66-8 CAPLUS

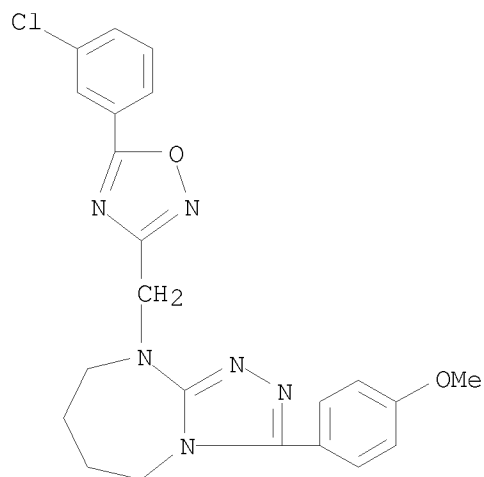
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(3-chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-3-(3,5-difluorophenyl)-6,7,8,9-tetrahydro- (CA INDEX NAME)



RN 863307-68-0 CAPLUS

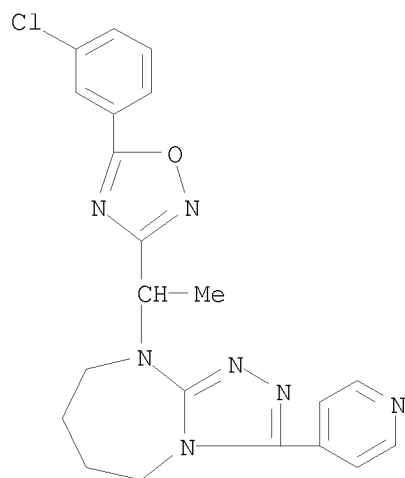
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(3-chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-6,7,8,9-tetrahydro-3-(4-methoxyphenyl)- (CA INDEX NAME)

10/588,699



RN 863307-69-1 CAPLUS

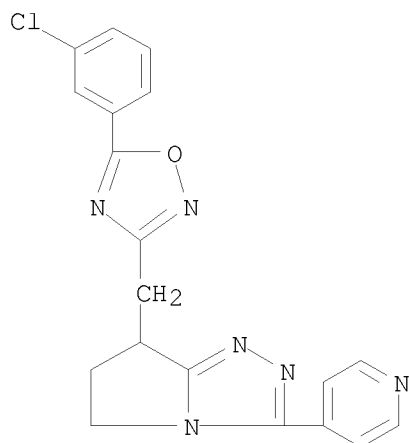
CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[1-[5-(3-chlorophenyl)-1,2,4-oxadiazol-3-yl]ethyl]-6,7,8,9-tetrahydro-3-(4-pyridinyl)- (CA INDEX NAME)



RN 863307-70-4 CAPLUS

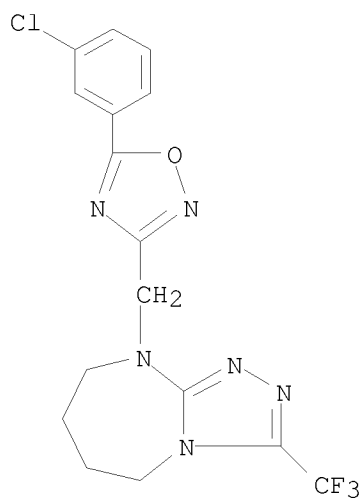
CN 5H-Pyrrolo[2,1-c]-1,2,4-triazole, 7-[[5-(3-chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-6,7-dihydro-3-(4-pyridinyl)- (CA INDEX NAME)

10/588,699



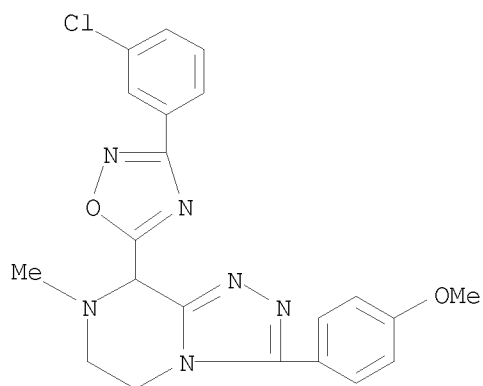
RN 863307-71-5 CAPLUS

CN 5H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 9-[[5-(3-chlorophenyl)-1,2,4-oxadiazol-3-yl]methyl]-6,7,8,9-tetrahydro-3-(trifluoromethyl)- (CA INDEX NAME)

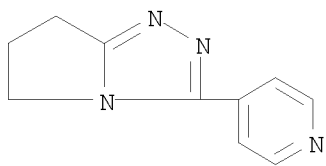


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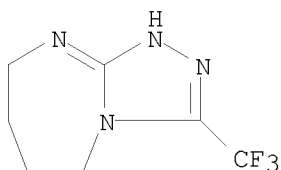
CN 1,2,4-Triazolo[4,3-a]pyrazine, 8-[3-(3-chlorophenyl)-1,2,4-oxadiazol-5-yl]-5,6,7,8-tetrahydro-3-(4-methoxyphenyl)-7-methyl- (CA INDEX NAME)



IT 114722-58-6P, 3-(Pyridin-4-yl)-6,7-dihydro-5H-pyrrolo[2,1-c][1,2,4]triazole 148461-26-1P, 3-(Trifluoromethyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 775260-07-6P, 3-(Pyridin-4-yl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-49-7P, 3-(3,5-Difluorophenyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-50-0P, 3-(4-Methoxyphenyl)-6,7,8,9-tetrahydro-5H-[1,2,4]triazolo[4,3-a][1,3]diazepine 863307-57-7P, 8-[3-(3-Chlorophenyl)-[1,2,4]oxadiazol-5-yl]-3-(4-methoxyphenyl)-5,6-dihydro-8H-[1,2,4]triazolo[4,3-a]pyrazine-7-carboxylic acid tert-butyl ester  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of heterocyclic-fused 1,3-diazenes and analogs as metabotropic glutamate receptor antagonists)  
 RN 114722-58-6 CAPLUS  
 CN 5H-Pyrrolo[2,1-c]-s-triazole, 6,7-dihydro-3-(4-pyridinyl)- (6CI, 9CI) (CA INDEX NAME)



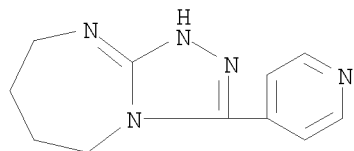
RN 148461-26-1 CAPLUS  
 CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 5,6,7,8-tetrahydro-3-(trifluoromethyl)- (CA INDEX NAME)



10/588,699

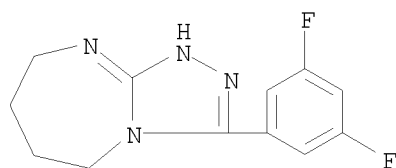
RN 775260-07-6 CAPLUS

CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 5,6,7,8-tetrahydro-3-(4-pyridinyl)-  
(CA INDEX NAME)



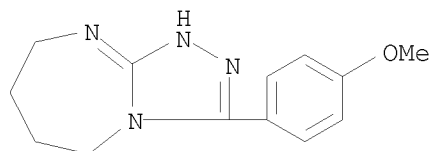
RN 863307-49-7 CAPLUS

CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 3-(3,5-difluorophenyl)-5,6,7,8-tetrahydro- (CA INDEX NAME)



RN 863307-50-0 CAPLUS

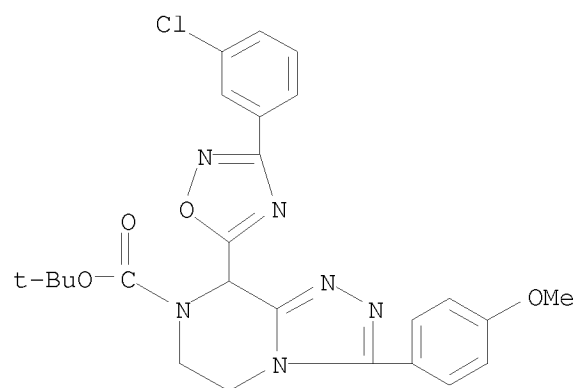
CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 5,6,7,8-tetrahydro-3-(4-methoxyphenyl)- (CA INDEX NAME)



RN 863307-57-7 CAPLUS

CN 1,2,4-Triazolo[4,3-a]pyrazine-7(8H)-carboxylic acid, 8-[3-(3-chlorophenyl)-1,2,4-oxadiazol-5-yl]-5,6-dihydro-3-(4-methoxyphenyl)-, 1,1-dimethylethyl ester (CA INDEX NAME)

10/588,699





L17 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:962228 CAPLUS

DOCUMENT NUMBER: 143:266932

TITLE: Preparation of tetrazole compounds and their use as metabotropic glutamate receptor antagonists

INVENTOR(S): Johansson, Martin; Minidis, Alexander; Staaf, Karin; Wensbo, David; McLeod, Donald; Edwards, Louise; Isaac, Methvin; O'Brien, Anne; Slassi, Abdelmalik; Xin, Tao

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; NPS Pharmaceuticals, Inc.

SOURCE: PCT Int. Appl., 118 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

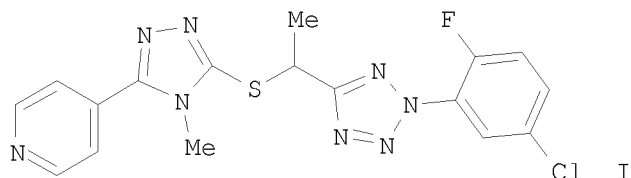
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005080356	A1	20050901	WO 2005-US5217	20050217
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005214379	A1	20050901	AU 2005-214379	20050217
CA 2556263	A1	20050901	CA 2005-2556263	20050217
EP 1716125	A1	20061102	EP 2005-713793	20050217
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, BA, HR, IS, YU				
CN 1918137	A	20070221	CN 2005-80004370	20050217
BR 2005007498	A	20070710	BR 2005-7498	20050217
JP 2007523182	T	20070816	JP 2006-554236	20050217
US 20060004021	A1	20060105	US 2005-60463	20050218
NO 2006003470	A	20061117	NO 2006-3470	20060728
IN 2006DN04470	A	20070810	IN 2006-DN4470	20060802
KR 2007027504	A	20070309	KR 2006-715943	20060807
MX 2006PA09019	A	20070308	MX 2006-PA9019	20060808
US 20070197549	A1	20070823	US 2007-588756	20070309
PRIORITY APPLN. INFO.:			US 2004-545291P	P 20040218
			WO 2005-US5217	W 20050217

OTHER SOURCE(S): MARPAT 143:266932

GI



AB The present invention relates to new tetrazole compds., or salts, solvates or solvated salts thereof, processes for their preparation and new intermediates used in the preparation thereof, pharmaceutical compns.

containing

said compds., and to the use of said compds. in therapy. E.g., I was prepared from 1-[2-(5-chloro-4-phenyl)-2H-tetrazol-5-yl]ethyl methanesulfonate, K<sub>2</sub>CO<sub>3</sub>, and 4-methyl-5-pyridin-4-yl-2,4-dihydro-[1,2,4]triazole-3-thione in MeCN. IC<sub>50</sub> values for glutamate receptor assays were given for I and Et 4-[1-[2-(3-chlorophenyl)-2H-tetrazol-5-yl]ethyl]piperazine-1-carboxylate.

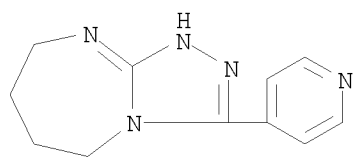
IT 775260-07-6P 863307-49-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tetrazole compds. and their use as metabotropic glutamate receptor antagonists)

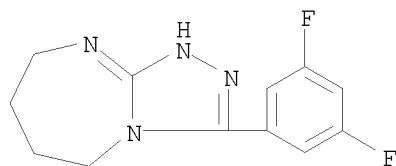
RN 775260-07-6 CAPLUS

CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 5,6,7,8-tetrahydro-3-(4-pyridinyl)- (CA INDEX NAME)



RN 863307-49-7 CAPLUS

CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 3-(3,5-difluorophenyl)-5,6,7,8-tetrahydro- (CA INDEX NAME)



REFERENCE COUNT:

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:449358 CAPLUS

DOCUMENT NUMBER: 119:49358

ORIGINAL REFERENCE NO.: 119:8957a,8960a

TITLE: Synthesis of 1,2,4-triazolo[4,3-a](1,3)diazepines.  
 Reactions of hexahydro-1H-1,3-diazepin-2-one hydrazone hydroiodide with acyl reagents. Part 7:  
 1,2,4-triazolo[4,3-a]diazacycloalkanes

AUTHOR(S): Krezel, Izabella

CORPORATE SOURCE: Dep. Pharm. Chem. Drug Anal., Med. Acad., Lodz, Pol.

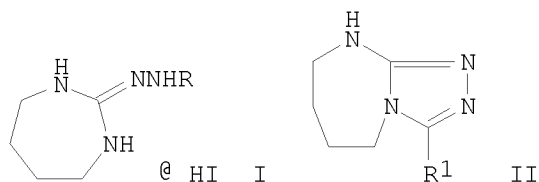
SOURCE: Pharmazie (1993), 48(3), 189-92

CODEN: PHARAT; ISSN: 0031-7144

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



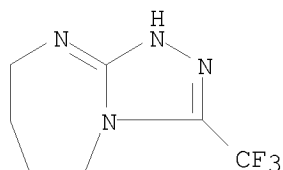
AB Reactions of hexahydro-1H-1,3-diazepin-2-one hydrazone hydroiodide I (R = H) with different acyl reagents are described. Reaction of I with R1COCl (R1 = Ph, 2-thienyl, CF3, PhCH2, etc.) affords, in acetonitrile, I (R = COR1), while in pyridine, the reaction products are derivs. of 1,2,4-triazolo[4,3-a](1,3)diazepines II. From the reaction of I (R = H) with trifluoroacetic anhydride, a mixture of I (R = COCF3) and II (R1 = CF3) was obtained. With acetic anhydride and I (R = H), acetyltriazolodiazepine III was obtained, while the reaction with trifluoroacetic acid affords, depending on reaction conditions, I (R = COCF3) or II (R1 = CF3).

IT 148461-26-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)

RN 148461-26-1 CAPLUS

CN 1H-1,2,4-Triazolo[4,3-a][1,3]diazepine, 5,6,7,8-tetrahydro-3-(trifluoromethyl)- (CA INDEX NAME)



L17 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 1961:38138 CAPLUS  
 DOCUMENT NUMBER: 55:38138  
 ORIGINAL REFERENCE NO.: 55:7450h-i,7451a-e  
 TITLE: 1,2,4-Triazole derivatives  
 PATENT ASSIGNEE(S): Farbenfabriken Bayer Akt.-Ges.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 825514		19591216	GB 1956-36166	19561126

GI For diagram(s), see printed CA Issue.

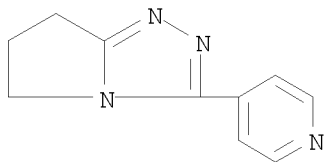
AB Triazole derivs., CH<sub>2</sub>.(CH<sub>2</sub>)<sub>n</sub>.N.N.C:N.N:CR (I), useful as analeptics and as central nervous system and respiratory system stimulants, were prepared from CH<sub>2</sub>.(CH<sub>2</sub>)<sub>n</sub>.C(OMe):N (II) and appropriate hydrazides. II (n = 4) (45 g.) added dropwise to 48.3 g. p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONHNH<sub>2</sub> in 500 g. hot alc., the mixture refluxed 1 hr., and filtered gave p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>CONHNH-C:N.(CH<sub>2</sub>)<sub>4</sub>.CH<sub>2</sub> (III), m. 188-97°. III (50 g.) heated with 200 g. AcOH and diluted with H<sub>2</sub>O gave 30% I (n = 4, R = p-O<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>), m. 184-5° [MeOCH<sub>2</sub>CH<sub>2</sub>OAc (IV)]. Hydrogenation of this compound gave I (n = 4, R = p-H<sub>2</sub>NC<sub>6</sub>H<sub>4</sub>), m. 210-12°. Compds. prepared similarly were:  
 CH:CH.N:CH.CH:CCONHNHC:N.(CH<sub>2</sub>)<sub>4</sub>.CH<sub>2</sub>, m. 208-10°; I (n = 4, R = 4-pyridyl) hydrochloride, m. 248-55° (sinters at 245°);  
 CH:N.CH:CH.CH:CCONHNHC:N.(CH<sub>2</sub>)<sub>4</sub>.CH<sub>2</sub>, m. 107-8° (from IV); and I (n = 4, R = 3-pyridyl), m. 81-2° (from IV). Prepared from II (n = 4) and the appropriate hydrazide without isolation of the intermediate were the following I (n = 4, R and m.p. given): H, about 65° (b16 239-41°; hydrochloride, m. 228-30°); NCCH<sub>2</sub>, 112-13° (hydrochloride, m. 253-5°); MeOCH<sub>2</sub>, - (hydrochloride, m. 156-8°); Ph, 132-4°; p-ClC<sub>6</sub>H<sub>4</sub>, 171° (from IV); 2,4-Cl<sub>2</sub>C<sub>6</sub>H<sub>3</sub>, 130-2° (EtOAc); p-MeOC<sub>6</sub>H<sub>4</sub>, 157-9°; o-HOC<sub>6</sub>H<sub>4</sub>, 260-5° (HCONMe<sub>2</sub>); α-furyl, 151-3° (EtOAc); H<sub>2</sub>NCO, 189-90° (hydrochloride decomposed at 245°); o-MeOC<sub>6</sub>H<sub>4</sub>, 160-1° (alc.); and 3-hydroxy-2-naphthyl, 306-8°. II (n = 4) and H<sub>2</sub>NNHCSNHNHCSOEt gave I (n = 4, R = NHNHCSOMe), m. 198-200°. II (n = 4) and (H<sub>2</sub>NNHCOCH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub> gave butylenebis I derivative (n = 4), m. 139-41°. Similarly the following I (n = 2) were prepared from II (n = 2) and the appropriate hydrazide (R and m.p. given): H (V), 65° (b0.6 200-2°; hydrochloride, m. 195-7°); H<sub>2</sub>NCO, 182-3°; 4-pyridyl (VI), -; butylenebis compound, 247-9° (H<sub>2</sub>O). OHCNHNH-C:N.(CH<sub>2</sub>)<sub>2</sub>.CH<sub>2</sub> and CH:CH.N:CH.CH:CHCONHNH-C:N.(CH<sub>2</sub>)<sub>2</sub>.CH<sub>2</sub>, intermediates in the preparation of V and VI, m. 138-40° and 127-8°, resp. II (n = 3) and (H<sub>2</sub>NNHCOCH<sub>2</sub>CH<sub>2</sub>)<sub>2</sub> gave 80-90% butylenebis I derivs. (n = 3), m. 185-6° (from IV). II (n = 3) and CH:CH.N:CH.CH:-CCONHNH<sub>2</sub> gave 90% I (n = 3, R = 4-pyridyl), m. 165-6°. Similarly II (n = 6) and the appropriate hydrazide gave I (n = 6, R = H), I (n = 6, R = H<sub>2</sub>NCO), m. 176-8°, and I (n = 6, R = 4-pyridyl), m. 117-19° (C<sub>6</sub>H<sub>6</sub>) [hydrochloride, m. 115-17° (H<sub>2</sub>O)].

IT 114722-58-6P, 5H-Pyrrolo[2,1-c]-s-triazole, 6,7-dihydro-3-(4-pyridyl)-  
 RL: PREP (Preparation)  
 (preparation of)

RN 114722-58-6 CAPLUS

10/588,699

CN 5H-Pyrrolo[2,1-c]-s-triazole, 6,7-dihydro-3-(4-pyridinyl)- (6CI, 9CI) (CA  
INDEX NAME)

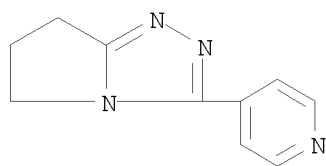


L17 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1960:50526 CAPLUS  
 DOCUMENT NUMBER: 54:50526  
 ORIGINAL REFERENCE NO.: 54:9960e-i,9961a  
 TITLE: Cycloalkanotriazoles and intermediates  
 INVENTOR(S): Petersen, Siegfried; Tietze, Ernst; Wirth, Wolfgang  
 PATENT ASSIGNEE(S): Schenley Industries, Inc.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Unavailable  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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	US 2913454		19591117	US 1956-623828	19561123
GI	For diagram(s), see printed CA Issue.				
AB	<p>The title compds. are prepared by treating a cyclic lactim ether of 5-10 C atoms with an acylhydrazine at 0-150°. They are useful as analeptics, stimulants, for the central nervous and respiratory systems, and intermediates in various syntheses. Thus, over 0.5 hr. caprolactim O-methyl ether 140 is added at 20°, without cooling, to monoformylhydrazine 60, in MeOH 400 parts (the temperature rises to 55°). After the mixture reaches 25°, it is refluxed on a H2O-bath 15 hrs., MeOH and H2O are distilled in vacuo at 100°, and the residue is distilled in vacuo from a metal bath to yield 4,5-pentamethylene-1,2,4-triazole 129 parts (94%), b16 239-41°, m. approx. 65° (hygroscopic colorless crystals); hydrochloride, m. 228-30° (decomposition). The following compds. are also prepared: 3-methoxymethyl-4,5-pentamethylene-1,2,4-triazole, b15 225-8°, viscous colorless oil; hydrochloride m. 156-8°; 3-phenyl-4,5-pentamethylene-1,2,4-triazole, brown crystals m. 132-4°; 3-(4-nitrophenyl)-4,5-pentamethylene-1,2,4-triazole, pale yellow crystals, m. 184-5°, prepared by ring closure of the intermediate m. 188-97°; 3-(o-hydroxyphenyl)-4,5-pentamethylene-1,2,4-triazole m. 260-5°; 3-(4-pyridyl)-4,5-pentamethylene-1,2,4-triazole, deliquescent crystals whose hydrochloride sinters at 245° and m. 248-55° and which is prepared from the intermediate 2-(2-benzoylhydrazino)-1-aza-1-cycloheptene, m. 208-10°; 3-(2-furyl)-4,5-pentamethylene-1,2,4-triazole, m. 151-3°; 3-carbamoyl-4,5-pentamethylene-1,2,4-triazole, m. 189-90°; hydrochloride decomposing at 245°; 3-(2-ethoxythiocarbonylhydrazino)-4,5-pentamethylene-1,2,4-triazole, needles, m. 198-200°; 3-cyanomethyl-4,5-pentamethylene-1,2,4-triazole, m. 112-13°; hydrochloride m. 253-5° (decomposition); 1,4-bis(4,5-tetramethylene-1,2,4-triazol-3-yl)butane, m. 139-41°; 4,5-tetramethylene-3-methyl-1,2,4-triazole, b14 224°, m. 85-6° (monohydrate m. 54-5°); 4,5-heptamethylene-1,2,4-triazole, viscous oil; 2-(2-methoxyhydrazino)-3,4,5,6,7-pentahydroazepine; 2-thiosemicarbazido-3,4,5,6,7-pentahydroazepine; and 2-(2-benzenesulfonylhydrazino)-3,4,5,6,7-pentahydroazepine.</p>				
IT	114722-58-6P, 5H-Pyrrolo[2,1-c]-s-triazole, 6,7-dihydro-3-(4-pyridyl)-				
	RL: PREP (Preparation)				
	(preparation of)				
RN	114722-58-6 CAPLUS				
CN	5H-Pyrrolo[2,1-c]-s-triazole, 6,7-dihydro-3-(4-pyridinyl)- (6CI, 9CI) (CA INDEX NAME)				

10/588,699



L17 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:50690 CAPLUS  
 DOCUMENT NUMBER: 52:50690  
 ORIGINAL REFERENCE NO.: 52:9158a-i,9159a-c  
 TITLE: Reactions of cyclic lactim ethers with acylhydrazine derivatives  
 AUTHOR(S): Petersen, Siegfried; Tietze, Ernst  
 CORPORATE SOURCE: Farbenfabrik Bayer, Leverkusen, Germany  
 SOURCE: Chemische Berichte (1957), 90, 909-21  
 CODEN: CHBEAM; ISSN: 0009-2940  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Unavailable  
 OTHER SOURCE(S): CASREACT 52:50690

GI For diagram(s), see printed CA Issue.

AB The previously reported (Schlack, C.A. 39, 14201)  $\text{H}_2\text{C}(\text{CH}_2)_4\text{N:COMe}$  (I) (30 g.) added to 20 g.  $\text{H}_2\text{NNHC:N:N:NH}$  in 250 cc. EtOH at  $50^\circ$ , boiled 30 min. on an H<sub>2</sub>O bath, and filtered hot yielded 31 g.  $\text{H}_2\text{C}(\text{CH}_2)_4\text{N:CR}$  (II) (R =  $\text{NHNHC:N:N:NH}$ ), m.  $225^\circ$  (decomposition) (H<sub>2</sub>O), with MeOH splitting off. I (30 g.) in 300 cc. EtOH similarly treated at  $60^\circ$  with 39.4 g.  $\text{o-C}_6\text{H}_4\text{SO}_2\text{N:CNHNH}_2$  yielded 26 g. II (R =  $\text{o-C}_6\text{H}_4\text{SO}_2\text{N:CNHNH}$ ), m.  $197-8^\circ$  ( $\text{HCONMe}_2\text{-H}_2\text{O}$ ), whereas 30 g. I with 32.8 g.  $\text{H}_2\text{NN.CH:N:N:CH}$  in 250 cc. EtOH needed 10 hrs. heating in an autoclave at  $140^\circ/10$  atmospheric to yield 35 g. II (R =  $\text{HNN.CH:N:N:CH}$ ), m.  $242^\circ$ . With  $\text{R'CONHNH}_2$  (III) I gave II (R =  $\text{R'CONHNH}$ ) (IV) as above, or by splitting off H<sub>2</sub>O from the enol form of IV  $\text{H}_2\text{C}(\text{CH}_2)_4\text{N.C:N:N:CR'}$  (V). Thus, 45 g. I added to 48.3 g. III (R' =  $4\text{-O}_2\text{NC}_6\text{H}_4$ ) in 500 cc. MeOH at  $60^\circ$  and boiled 1 hr. yielded 65 g. IV (R' =  $4\text{-O}_2\text{NC}_6\text{H}_4$ ) (VI), m.  $188^\circ$ ; and similarly I with III (R' =  $4\text{-pyridyl}$ ) gave IV (R' =  $4\text{-pyridyl}$ ) (VII), m.  $210^\circ$ . However, 140 g. I added dropwise to 60 g. III (R' = H) in 400 cc. MeOH at  $20^\circ$  during 30 min. while the temperature rose to  $55^\circ$ , the mixture refluxed 15 hrs., and distilled in vacuo yielded 129 g. V (R' = H), b<sub>16</sub>  $239-41^\circ$ , m.  $65^\circ$ ; HCl salt, m.  $228-30^\circ$ . Likewise, I with III (R' =  $\text{NCCH}_2$ , Ph, or  $2\text{-furyl}$ ) gave V (R' =  $\text{NCCH}_2$ , Ph, or  $2\text{-furyl}$ ), m.  $111^\circ$  (HCl salt, m.  $244^\circ$ ),  $133^\circ$ , and  $152^\circ$ , resp. That V were formed through IV was proved by obtaining both IV and V from a single compound in many cases, IV at lower temperature and shorter reaction time.

Thus,

50.8 g. I added dropwise to 29.6 g. III (R' = Me) in 200 cc. MeOH at  $0-5^\circ$  with stirring (1 hr.) and kept 15 hrs. at  $0^\circ$  yielded 45 g. IV (R' = Me), m.  $176-7^\circ$  (decomposition) (HCl salt, m.  $181^\circ$ ); 74 g. III (R' = Me) in 500 cc. MeOH and 140 g. I quickly mixed without cooling, refluxed 15 hrs., and distilled in vacuo yielded 133 g. V (R' = Me), b<sub>16</sub>  $235-7^\circ$ , m.  $108^\circ$  (HCl salt, m.  $213-15^\circ$ ), formed also by refluxing IV (R' = Me) 15 hrs. in MeOH. Likewise, 50 g. VI boiled 5 min. in 200 cc. AcOH, cooled to  $80^\circ$ , and 200 cc. H<sub>2</sub>O added yielded 40 g. V (R' =  $\text{O}_2\text{NC}_6\text{H}_4$ ), m.  $184^\circ$ . This ease of ring closure was shown by the catalytic reduction (Raney Ni) of 50 g. VI whereby 45 g. V (R' =  $\text{H}_2\text{NC}_6\text{H}_4$ ) was formed [not IV (R' =  $\text{H}_2\text{NC}_6\text{H}_4$ )], m.  $211^\circ$ , also formed by the catalytic reduction of V (R' =  $\text{O}_2\text{NC}_6\text{H}_4$ ). VII was also converted to the corresponding V (HCl salt, m.  $248-55^\circ$ ) by boiling 5 min. in AcOH. Other similar compds. were prepared (compound, R', and m.p. given): IV, Et,  $169^\circ$ ; IV,  $3\text{-pyridyl}$ ,  $108^\circ$ ; V, Et,  $41^\circ$  (b<sub>0.05</sub>  $164^\circ$ ); V,  $\text{H}_2\text{NCO}$ ,  $191^\circ$ ; V,  $\text{MeOCH}_2$ , b<sub>15</sub>  $226^\circ$  (HCl salt, m.  $157^\circ$ ); V,  $p\text{-ClC}_6\text{H}_4$ ,  $171^\circ$ ; V,  $2,4\text{-Cl}_2\text{C}_6\text{H}_3$ ,  $131^\circ$ ; V,  $\text{o-HOC}_6\text{H}_4$ ,  $260-5^\circ$ ; V,  $\text{o-MeOC}_6\text{H}_4$ ,  $161^\circ$ ; V,  $p\text{-MeOC}_6\text{H}_4$ ,  $158^\circ$ ; V,  $2,3\text{-HOC}_6\text{H}_6$ ,  $309^\circ$ ; V,



3-pyridyl, 81°. Noteworthy were the reactions of I with  $(\text{CH}_2)_4(\text{CONHNH}_2)_2$ ,  $\text{H}_2\text{NNHCO}_2\text{Et}$ ,  $\text{H}_2\text{NNHCSNH}_2$ ,  $\text{H}_2\text{NNHSO}_2\text{Ph}$ , and  $\text{H}_2\text{NNHCSNHNHCSOEt}$  under conditions similar to the preceding to give, resp.: bis V compound [ $\text{R}' = (\text{CH}_2)_4$ ], m. 140°; IV ( $\text{R}' = \text{CO}_2\text{Et}$ ), m. 122°, and then by longer heating and splitting off of EtOH instead of  $\text{H}_2\text{O}$ , V ( $\text{R}' = \text{HO}$ ), m. 179°; IV ( $\text{R}' = \text{CSNH}_2$ ), m. 240-50° (decomposition); IV ( $\text{R}' = \text{SO}_2\text{Ph}$ ), m. 190-1°; and V ( $\text{R}' = \text{NHNHCSOEt}$ ), m. 198-200°.

Finally it was found that  $\text{H}_2\text{C}(\text{CH}_2)_x\text{N:COMe}$  (VIII) ( $x = 2, 3$ , or  $6$ ) reacted as I did. According to Benson and Cairns (C.A. 42, 6749e) 252 g.  $\text{Me}_2\text{SO}_4$  added dropwise with stirring to 170 g.  $\text{H}_2\text{C}(\text{CH}_2)_x\text{N:COH}$  (IX) ( $x = 2$ ) in 100 cc.  $\text{C}_6\text{H}_6$  at 60-70°, the mixture refluxed 8 hrs., cooled to 5°, 150 g.  $\text{K}_2\text{CO}_3$  quickly added, then 100 cc.  $\text{H}_2\text{O}$  added dropwise with cooling (1 hr.) while  $\text{CO}_2$  evolved and the temperature rose to 20°, and the  $\text{C}_6\text{H}_6$  layer distilled in vacuo yielded 95 g. VIII ( $x = 2$ ), b. 118-21°, rearranged by heating 1-2 hrs. at 120-5° to  $\text{H}_2\text{C}(\text{CH}_2)_x\text{NMe.CO}$  (X) ( $x = 2$ ), b. 198-200°, b12 82-3°. Similar treatment converted IX ( $x = 6$ ) at 75% VIII ( $x = 6$ ), b14 89°, b0.1 61-2°, rearranged to X ( $x = 6$ ), b14 140°.

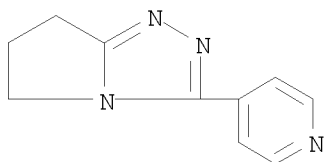
$\text{R}'$  and m.p. (in parentheses) for IV prepared from VIII ( $x = 2$ ) were: H (139°), Me (194°), EtO (151°), 4-pyridyl (227°). For V prepared from VIII ( $x = 2$ ): H (HCl salt, m. 196°), Me (HCl salt, m. 200°), HO (179°),  $\text{H}_2\text{NCO}$  (181°), 4-pyridyl (186°),  $(\text{CH}_2)_4$  (bis V compound) (247°). For IV prepared from VIII ( $x = 6$ ): EtO (132°). For V prepared from VIII ( $x = 3$ ): Me (86°) (b14 224°), HO (131°), 4-pyridyl (166°),  $(\text{CH}_2)_4$  (bis V compound) (184°). For V prepared from VIII ( $x = 6$ ): H (b0.1 167°), Me (40°) (b0.6 172°) (HCl salt, m. 168°), HO (112°),  $\text{H}_2\text{NCO}$  (177°),  $\text{MeOCH}_2$  (b0.2 188°), Ph (113°), 3-pyridyl (104°), 4-pyridyl (119°) (HCl salt, m. 216°),  $(\text{CH}_2)_4$  (bis V compound) (112°).

IT 114722-58-6P, 5H-Pyrrolo[2,1-c]-s-triazole, 6,7-dihydro-3-(4-pyridyl)-

RL: PREP (Preparation)  
(preparation of)

RN 114722-58-6 CAPLUS

CN 5H-Pyrrolo[2,1-c]-s-triazole, 6,7-dihydro-3-(4-pyridinyl)- (6CI, 9CI) (CA INDEX NAME)



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